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Biomolecular dynamics by computer analysis

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Abstract: As numerical tools (computers and display equipment) become more powerful and the atomic structures of important biological molecules become known, the importance of detailed computation of nonequilibrium biomolecular dynamics increases. In this note we briefly report results from a well developed study of the hydrogen bonded polypeptide crystal acetanilide, a model protein. Extensions to other areas of molecular dynamics are also surveyed.

It is over ten years since Davydov [1] first suggested a self-trapping mechanism in α-helix proteins which would give rise to a soliton-like excitation on these biologically important molecules. This pioneering work has led to extensive theoretical and experimental investigations on both sides of the Atlantic. In this note we summarize some of the work we have carried out in this area. Since full details of the topics discussed here have or will be published elsewhere, we give only a brief introductory sketch and refer the reader to the bibliography for details. In particular we have added some references to work done since the conference at which this paper was originally given.

The study began with an investigation into solitons in acetanilide (ACN), a crystalline material with many properties in common with α-helix proteins [2,3]. The work extended in a natural manner to a theory of self-trapping, applicable to many discrete systems, described by a new set of equations which we have called the Discrete Self-Trapping (DST) equation [4]. This equation has the form

$$\mathrm{i}\dot{\boldsymbol{A}} + \gamma \begin{bmatrix} |A_1|^2 & & & 0 \\ & |A_2|^2 & & \\ & & \ddots & \\ 0 & & & |A_n|^2 \end{bmatrix} \boldsymbol{A} + \epsilon \boldsymbol{M}\boldsymbol{A} = 0 \tag{1}$$

where $\boldsymbol{A}$ is a complex n-vector, γ and ϵ are real parameters, and $\boldsymbol{M}$ is an arbitrary real symmetric $n \times n$ matrix.

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In the ACN model, A_i is probability amplitude for a quanta on the ith amide-I bond, γ is a measure of the nonlinearity of the hydrogen bonds joining the amide groups, and ϵM is an interaction term describing the dipole coupling between different sites in the molecule. Although this equation was developed to describe solitons on large discrete lattices, it turns out that the same equation has important applications to solitons on α-helix proteins or globular proteins [6], and polarons in a crystal [7]. For a small number of lattice sites (small n), (1) has been used as a simple model for vibrational states of polyatomic molecultes [5]. If M is chosen to be tridiagonal, with appropriately chosen coefficients, a finite difference version of the nonlinear Schrödinger (NLS) equation is obtained. Other applications and further references are given in a recent review [8].

In studying solutions of (1), some progress can be made by restricting the space of solutions to stationary solutions, i.e. those having the form $\boldsymbol{A}(t) = \phi \exp(\mathrm{i}\omega t)$, where ϕ is a time independent n-vector. Inserting this into (1) we get a nonlinear eigenvalue problem for ω and ϕ

$$-\omega\phi + \gamma \begin{bmatrix} |\phi_1|^2 & & & 0 \\ & |\phi_2|^2 & & \\ & & \ddots & \\ 0 & & & |\phi_n|^2 \end{bmatrix} \phi + \epsilon M \phi = 0. \tag{2}$$

Many analytic solutions of (2) have been found, especially for small n and interaction matrices M with high degrees of symmetry. Other more approximate solutions have been found by perturbation techniques and by numerical path following calculations. It is interesting to note that many of the exact analytical formulae were discovered only after the corresponding solution curve had been calculated numerically, and some simplifying relationship was noted from the computer output.

These stationary solutions are a useful starting point for the investigation of the full time-dependent DST equation (1). Except for the case $n = 2$, and for larger n the stationary solutions noted above, in general the only way to investigate full time-dependent solutions of (1) is numerically. Solutions of the full equation display the full spectrum of periodic, quasi-periodic and chaotic solutions now familiar in the study of dynamical systems: however the spatial structure of the chaotic solutions often appears as soliton-like solutions of (2) moving erratically in time [8,9].

Recent work has concentrated on a quantized version of the DST equation. Some interesting applications to classical and quantum descriptions of normal mode and local mode vibrational states have been made. One specific application has been to model local modes in benzine [9,10]. More generally, a number of results concerning the energy levels of local mode excitations have been discovered [11]. In systems with transitive symmetry, the degeneracy between different 'soliton' modes with m quanta in one mode can only be removed by going to mth order perturbation theory, and an exact formula for the splitting to this level of perturbation theory can be obtained. This is in contrast to the quantum mechanical treatment of coupled *linear* oscillators, where such local modes are completely degenerate with other modes in the system [12]. Again it is interesting to note that the exact formulae obtained in the nonlinear case were first obtained by numerical computer experiments before being proved analytically. Thus in all stages of this investigation, numerical results have suggested analytic properties to investigate,

and the analytic solutions have formed a background of known solutions which help to understand more complicated numerical results.

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